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Mo2C as a high capacity anode material: a first-principles study
DENIZ CAKIR, University of North Dakota, CEM SEVIK, Anadolu University, OGUZ GULSEREN, Bilkent University, FRANCOIS PEETERS, University of Antwerp — The adsorption and diffusion of Li, Na, K and Ca atoms on a Mo2C monolayer are investigated by using first principles methods. We found that the considered metal atoms are strongly bound to the Mo2C monolayer. However, the adsorption energies of these alkali and earth alkali elements decreases as coverage increases due to the enhanced repulsion between the metal ions. We predict a significant charge transfer from the ad-atoms to the Mo2C monolayer, which indicates clearly the cationic state of the metal atoms. The metallic character of both pristine and doped Mo2C ensures a good electronic conduction. Low migration energy barriers are predicted as small as 43 meV for Li, 19 meV for Na and 15 meV for K, which result in the very fast diffusion of these atoms on Mo2C. For Mo2C, we found a store capacity larger than 400 mAh/g by the inclusion of multilayer adsorption. Mo2C expands slightly upon deposition of Li and Na even at high concentrations, which ensures a good cyclic stability of the atomic layer. The calculated average voltage of 0.68 V for Li and 0.30 V for Na ions makes Mo2C attractive for low charging voltage applications. D. Cakır, C. Sevik, O. Gulseren and F. M. Peeters, J. Mater. Chem. A 4, 6029 (2016).

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